

N-Butyl-6-chloro-3-hydrazinylpyridazin-4-amine
61261-44-7 | DTXSID70615443

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 138 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.87e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Atrazine</div> <div>Measured: 174</div> <div>Predicted: 202</div>	<div>Image not found</div> <div>Simazine</div> <div>Measured: 126</div> <div>Predicted: 135</div>	<div>Image not found</div> <div>Simetone</div> <div>Measured: 219</div> <div>Predicted: 218</div>
<div>Image not found</div> <div>Dimethyl phthalate</div> <div>Measured: 39.8</div> <div>Predicted: 59.9</div>	<div>Image not found</div> <div>Propazine</div> <div>Measured: 251</div> <div>Predicted: 280</div>	